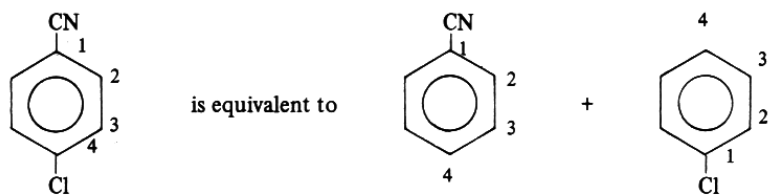


¹³C – NMR Chemical Shift Increments for substituted benzenes



	Calcd.	Observed	Observed	Observed
1.	-17.3	-16.6	1. -15.4	4. -1.9
2.	+ 4.9	+ 5.1	2. + 3.6	3. +1.3
3.	+ 1.0	+ 1.3	3. + 0.6	2. +0.4
4.	+10.1	+10.8	4. + 3.9	1. +6.2

Table VII. Incremental Shifts of the Aromatic Carbon Atoms of Monosubstituted Benzenes (ppm from Benzene at 128.5 ppm, + downfield, – upfield). C Atom of Substituents in ppm from TMS

Substituent	C-1 (Attachment)	C-2	C-3	C-4	C of Substituent (ppm from TMS)
H ^b	0.0	0.0	0.0	0.0	
CH ₃ ^b	+8.9	+0.7	-0.1	-2.9	21.3
CH ₂ CH ₃ ^a	+15.6	-0.5	0.0	-2.6	29.2 (CH ₂), 15.8 (CH ₃)
CH(CH ₃) ₂ ^a	+20.1	-2.0	0.0	-2.5	34.4 (CH), 24.1 (CH ₃)
C(CH ₃) ₃ ^a	+22.2	-3.4	-0.4	-3.1	34.5 (C), 31.4 (CH ₃)
CH=CH ₂ ^a	+9.5	-2.0	+0.2	-0.5	135.5 (CH), 112.0 (CH ₂)
C≡CH ^b	-6.1	+3.8	+0.4	-0.2	
C ₆ H ₅ ^b	+13.1	-1.1	+0.4	-1.2	
CH ₂ OH ^a	+12.3	-1.4	-1.4	-1.4	64.5
CH ₂ OCCH ₃ ^c	+7.7	~0.0	~0.0	~0.0	20.7 (CH ₃), 66.1 (CH ₂), 170.5 (C=O)
OH ^b	+26.9	-12.7	+1.4	-7.3	
OCH ₃ ^b	+31.4	-14.4	+1.0	-7.7	54.1
OC ₆ H ₅ ^a	+29.2	-9.4	+1.6	-5.1	
OCCH ₃ ^a	+23.0	-6.4	+1.3	-2.3	
CH ^a	+8.6	+1.3	+0.6	+5.5	192.0
CCH ₃ ^b	+9.1	+0.1	0.0	+4.2	25.0 (CH ₃), 195.7 (C=O)
CC ₆ H ₅ ^b	+9.4	+1.7	-0.2	+3.6	
CCF ₃ ^b	-5.6	+1.8	+0.7	+6.7	
COH ^b	+2.1	+1.5	0.0	+5.1	172.6
COCH ₃ ^a	+1.3	-0.5	-0.5	+3.5	51.0 (CH ₃)
CCl ^b	+4.6	+2.4	0.0	+6.2	
CO ^b	+21.9 (7.5 Hz)	-8.4 (5.0 Hz)	+1.2	-3.0	chemical shifts

Table VII (continued)

Substituent	C-1 (Attachment)	C-2	C-3	C-4	C of Substituent (ppm from TMS)
$\begin{array}{c} \text{O} \\ \parallel \\ \text{CCF}_3^b \end{array}$	-5.6	+1.8	-0.7	+6.7	118.7
$\text{C}\equiv\text{N}^b$	-15.4	+3.6	+0.6	+3.9	
NH_2^b	+18.0	-13.3	+0.9	-9.8	
$\text{N}(\text{CH}_3)_2^a$	+22.4	-15.7	+0.8	-15.7	
$\begin{array}{c} \text{O} \\ \parallel \\ \text{NHCCH}_3^a \end{array}$	+11.1	-9.9	+0.2	-5.6	129.5
NO_2^b	+20.0	-4.8	+0.9	+5.8	
$\text{N}=\text{C}=\text{O}^b$	+5.7	-3.6	+1.2	-2.8	
F^b	+34.8	-12.9	+1.4	-4.5	
Cl^b	+6.2	+0.4	+1.3	-1.9	
Br^b	-5.5	+3.4	+1.7	-1.6	
I^a	-32.2	+9.9	+2.6	-7.4	
CF_3^b	-9.0	-2.2	+0.3	+3.2	
SH^c	+2.3	+1.1	+1.1	-3.1	
SCH_3^c	+10.2	-1.8	+0.4	-3.6	
SO_2NH_2^c	+15.3	-2.9	+0.4	+3.3	
$\text{Si}(\text{CH}_3)_3^a$	+13.4	+4.4	-1.1	-1.1	

^aNeat^bIn CCl_4 ^cIn CDCl_3